

Carbazole-2-carbonitrile, 5,6,7,8-tetrahydro-1-methyl-
73771-63-8 | DTXSID50224153

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 20.0

Global applicability domain: Inside

Local applicability domain index: 4.54e-01

Confidence level: 5.77e-01

Nearest Neighbors from the Training Set

Image not found

Molinate

Measured: 25.7

Predicted: 14.8

Image not found

N,N-Diethylaniline

Measured: 102

Predicted: 12.8

Image not found

4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69

Image not found

Isoamyl ether

Measured: 170

Predicted: 137